



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 03:34 PM EDT

PDB ID : 6NLG  
Title : 1.50 Å resolution structure of BfrB (C89S/K96C) from *Pseudomonas aeruginosa* in complex with a small molecule fragment (analog 1)  
Authors : Lovell, S.; Punchi-Hewage, A.; Battaile, K.P.; Yao, H.; Nammalwar, B.; Gnanasekaran, K.K.; Bunce, R.A.; Reitz, A.B.; Rivera, M.  
Deposited on : 2019-01-08  
Resolution : 1.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : **FAILED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

## 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6037 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

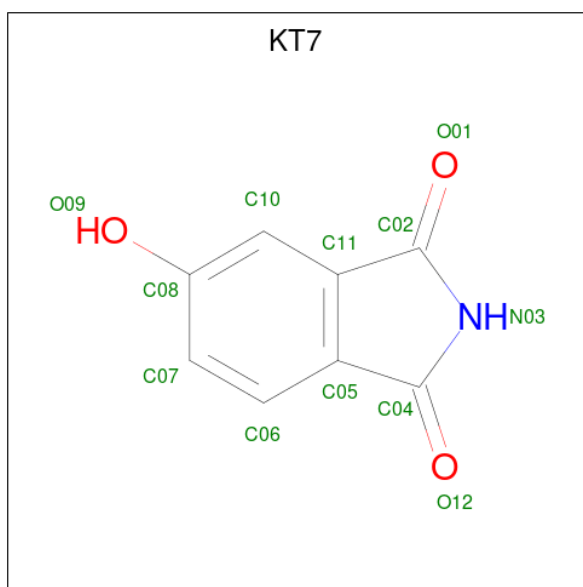
- Molecule 1 is a protein called Bacterioferritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	156	1315	833	218	256	8	0	9	0
1	B	156	1287	813	215	251	8	0	5	0
1	C	156	1307	827	218	253	9	0	7	0
1	D	156	1287	814	217	249	7	0	4	0

There are 8 discrepancies between the modelled and reference sequences:

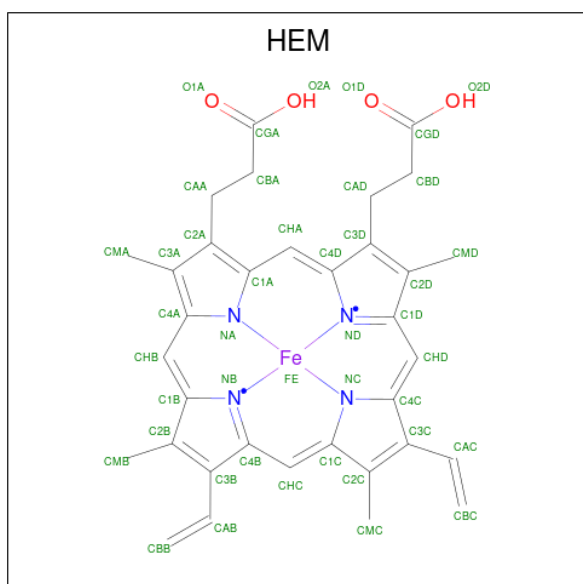
Chain	Residue	Modelled	Actual	Comment	Reference
A	89	SER	CYS	engineered mutation	UNP Q9HY79
A	96	CYS	LYS	engineered mutation	UNP Q9HY79
B	89	SER	CYS	engineered mutation	UNP Q9HY79
B	96	CYS	LYS	engineered mutation	UNP Q9HY79
C	89	SER	CYS	engineered mutation	UNP Q9HY79
C	96	CYS	LYS	engineered mutation	UNP Q9HY79
D	89	SER	CYS	engineered mutation	UNP Q9HY79
D	96	CYS	LYS	engineered mutation	UNP Q9HY79

- Molecule 2 is 5-hydroxy-1H-isoindole-1,3(2H)-dione (three-letter code: KT7) (formula:  $C_8H_5NO_3$ ).



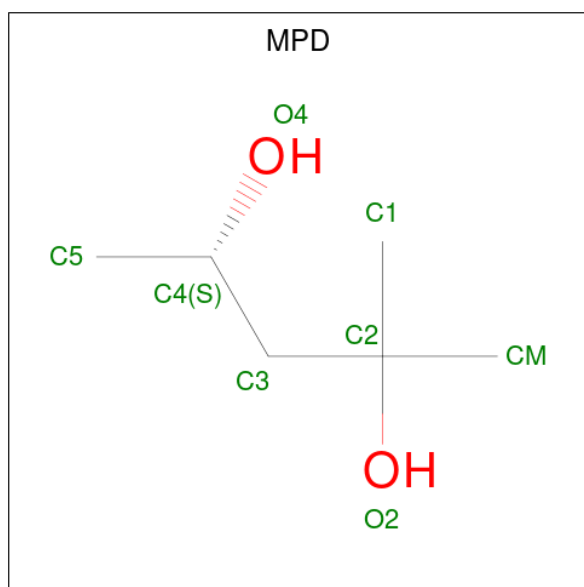
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			12	8	1	3		
2	C	1	Total	C	N	O	0	0
			12	8	1	3		
2	D	1	Total	C	N	O	0	0
			12	8	1	3		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total	C	Fe	N	O	0	1
			86	68	2	8	8		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C O	0	0
			8	6 2		
4	B	1	Total	C O	0	0
			8	6 2		
4	C	1	Total	C O	0	0
			8	6 2		
4	D	1	Total	C O	0	0
			8	6 2		

- Molecule 5 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 3 2 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total K 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	142	Total 142	O 142	0	0
7	B	140	Total 140	O 140	0	0
7	C	140	Total 140	O 140	0	0
7	D	125	Total 125	O 125	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

### 3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.81Å 153.81Å 153.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.35 – 1.50	Depositor
% Data completeness (in resolution range)	99.5 (38.35-1.50)	Depositor
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 1.50Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.150 , 0.158	Depositor
Wilson B-factor (Å <sup>2</sup> )	17.2	Xtrriage
Anisotropy	0.277	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6037	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.3 Torsion angles [i](#)

#### 4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 4.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 1 is monoatomic - leaving 22 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	HEM	A	202[B]	1	41,50,50	1.30	4 (9%)	45,82,82	1.80	8 (17%)
4	MPD	B	202	-	7,7,7	0.36	0	9,10,10	0.78	0
4	MPD	C	203	-	7,7,7	0.42	0	9,10,10	0.54	0
3	HEM	D	202	1	41,50,50	1.38	3 (7%)	45,82,82	1.66	12 (26%)
5	SO4	A	204	-	4,4,4	0.27	0	6,6,6	0.49	0
3	HEM	C	202	1	41,50,50	1.38	4 (9%)	45,82,82	1.48	7 (15%)
5	SO4	A	206	-	4,4,4	0.82	0	6,6,6	0.64	0
2	KT7	A	201	-	13,13,13	1.51	2 (15%)	19,19,19	1.50	4 (21%)
4	MPD	D	203	-	7,7,7	0.32	0	9,10,10	0.73	0
5	SO4	B	203	-	0,2,4	-	-	0,1,6	-	-
5	SO4	D	205	-	4,4,4	0.87	0	6,6,6	1.12	0
5	SO4	D	204	-	4,4,4	0.21	0	6,6,6	0.54	0
4	MPD	A	203	-	7,7,7	0.34	0	9,10,10	0.77	0
3	HEM	A	202[A]	1	41,50,50	1.30	4 (9%)	45,82,82	1.79	8 (17%)
5	SO4	A	207	-	4,4,4	0.61	0	6,6,6	0.29	0
2	KT7	D	201	-	13,13,13	1.56	3 (23%)	19,19,19	1.94	6 (31%)
5	SO4	C	206	-	4,4,4	0.16	0	6,6,6	0.21	0
2	KT7	C	201	-	13,13,13	1.43	3 (23%)	19,19,19	1.76	4 (21%)
5	SO4	C	204	-	4,4,4	0.09	0	6,6,6	0.17	0
5	SO4	B	204	-	4,4,4	0.11	0	6,6,6	0.35	0
5	SO4	A	205	-	4,4,4	0.17	0	6,6,6	0.30	0
5	SO4	C	205	-	4,4,4	0.23	0	6,6,6	0.38	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	A	202[B]	1	-	4/12/54/54	-
2	KT7	A	201	-	-	-	0/2/2/2
4	MPD	A	203	-	-	2/5/5/5	-
4	MPD	B	202	-	-	1/5/5/5	-
4	MPD	C	203	-	-	3/5/5/5	-
4	MPD	D	203	-	-	2/5/5/5	-
3	HEM	A	202[A]	1	-	4/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	KT7	C	201	-	-	-	0/2/2/2
3	HEM	D	202	1	-	4/12/54/54	-
3	HEM	C	202	1	-	4/12/54/54	-
2	KT7	D	201	-	-	-	0/2/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	202	HEM	C3C-C2C	-3.97	1.34	1.40
3	D	202	HEM	C3C-C2C	-3.72	1.35	1.40
3	D	202	HEM	C3C-CAC	3.40	1.54	1.47
2	A	201	KT7	C02-N03	3.29	1.43	1.38
3	A	202[B]	HEM	C1B-NB	-3.23	1.34	1.40
3	A	202[A]	HEM	C1B-NB	-3.19	1.34	1.40
3	A	202[B]	HEM	C4D-ND	-3.14	1.34	1.40
3	A	202[A]	HEM	C4D-ND	-3.11	1.34	1.40
3	A	202[A]	HEM	FE-NB	2.94	2.11	1.96
3	A	202[B]	HEM	FE-NB	2.94	2.11	1.96
2	D	201	KT7	C11-C02	2.83	1.52	1.48
2	C	201	KT7	C02-N03	2.75	1.42	1.38
3	C	202	HEM	C3C-CAC	2.74	1.53	1.47
2	A	201	KT7	C04-N03	2.73	1.42	1.38
3	D	202	HEM	CAB-C3B	2.66	1.54	1.47
2	D	201	KT7	C02-N03	2.60	1.42	1.38
2	C	201	KT7	C04-N03	2.49	1.42	1.38
2	D	201	KT7	C10-C11	2.38	1.43	1.39
3	C	202	HEM	CAB-C3B	2.25	1.53	1.47
2	C	201	KT7	C11-C02	2.22	1.52	1.48
3	A	202[B]	HEM	CHB-C1B	2.08	1.40	1.35
3	C	202	HEM	CMB-C2B	2.08	1.55	1.50
3	A	202[A]	HEM	CHB-C1B	2.06	1.40	1.35

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	202[B]	HEM	CHC-C4B-NB	5.14	130.02	124.43
3	A	202[A]	HEM	CHC-C4B-NB	5.13	130.00	124.43
2	D	201	KT7	C10-C11-C02	4.88	134.70	129.66
2	A	201	KT7	C04-N03-C02	-4.62	108.59	112.52
2	C	201	KT7	C04-N03-C02	-4.53	108.66	112.52
3	A	202[B]	HEM	CHD-C1D-ND	4.34	129.15	124.43
3	A	202[A]	HEM	CHD-C1D-ND	4.30	129.10	124.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	202	HEM	CMC-C2C-C3C	4.22	132.57	124.68
2	C	201	KT7	C10-C11-C02	4.10	133.90	129.66
3	D	202	HEM	CBA-CAA-C2A	-3.81	106.11	112.62
3	A	202[B]	HEM	C1B-NB-C4B	3.67	108.86	105.07
3	D	202	HEM	CMC-C2C-C3C	3.67	131.54	124.68
3	A	202[A]	HEM	C1B-NB-C4B	3.64	108.83	105.07
3	A	202[B]	HEM	CHA-C4D-ND	3.57	128.80	124.38
3	A	202[A]	HEM	CHA-C4D-ND	3.53	128.74	124.38
3	D	202	HEM	C4D-ND-C1D	3.48	108.67	105.07
2	D	201	KT7	C04-N03-C02	-3.41	109.62	112.52
3	A	202[B]	HEM	CHB-C1B-NB	3.38	128.56	124.38
3	A	202[A]	HEM	CHB-C1B-NB	3.36	128.53	124.38
3	C	202	HEM	CBA-CAA-C2A	-3.14	107.26	112.62
3	C	202	HEM	CMA-C3A-C4A	-3.12	123.67	128.46
2	C	201	KT7	C05-C04-N03	2.84	108.50	105.89
3	A	202[B]	HEM	CHD-C1D-C2D	-2.68	120.80	124.98
3	D	202	HEM	C4C-CHD-C1D	2.66	126.08	122.56
3	A	202[A]	HEM	CHD-C1D-C2D	-2.66	120.82	124.98
2	A	201	KT7	C10-C11-C02	2.65	132.40	129.66
2	D	201	KT7	C05-C04-N03	2.56	108.24	105.89
3	C	202	HEM	C4D-ND-C1D	2.46	107.61	105.07
3	D	202	HEM	C3B-C2B-C1B	2.40	108.27	106.49
2	D	201	KT7	C10-C11-C05	-2.39	118.50	121.83
3	D	202	HEM	C1B-NB-C4B	2.36	107.51	105.07
3	D	202	HEM	CAD-CBD-CGD	-2.34	108.57	113.60
2	C	201	KT7	C10-C11-C05	-2.29	118.64	121.83
3	D	202	HEM	C2D-C1D-ND	-2.25	107.18	109.88
3	A	202[B]	HEM	CHA-C4D-C3D	-2.25	121.11	125.33
3	A	202[A]	HEM	CHA-C4D-C3D	-2.24	121.11	125.33
3	D	202	HEM	C4B-CHC-C1C	2.21	125.48	122.56
2	D	201	KT7	O01-C02-C11	2.19	133.43	127.67
2	A	201	KT7	C11-C02-N03	2.18	107.90	105.89
3	C	202	HEM	C2C-C3C-C4C	2.18	108.42	106.90
3	D	202	HEM	C3D-C4D-ND	-2.17	107.75	110.17
3	D	202	HEM	CMA-C3A-C4A	-2.16	125.14	128.46
2	A	201	KT7	C05-C04-N03	2.14	107.86	105.89
3	A	202[B]	HEM	C4D-ND-C1D	2.12	107.26	105.07
2	D	201	KT7	O01-C02-N03	-2.11	119.07	125.56
3	D	202	HEM	CMB-C2B-C1B	-2.08	121.88	125.04
3	C	202	HEM	C4B-C3B-C2B	2.07	108.76	107.11
3	A	202[A]	HEM	C4D-ND-C1D	2.07	107.21	105.07
3	C	202	HEM	C4A-C3A-C2A	2.05	108.42	107.00

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	203	MPD	C2-C3-C4-C5
4	B	202	MPD	C2-C3-C4-C5
4	C	203	MPD	C2-C3-C4-O4
4	D	203	MPD	C2-C3-C4-C5
4	C	203	MPD	O2-C2-C3-C4
4	D	203	MPD	C2-C3-C4-O4
3	A	202[A]	HEM	CAD-CBD-CGD-O2D
3	D	202	HEM	CAA-CBA-CGA-O1A
3	D	202	HEM	CAA-CBA-CGA-O2A
3	C	202	HEM	CAA-CBA-CGA-O2A
3	D	202	HEM	CAD-CBD-CGD-O1D
3	A	202[B]	HEM	CAD-CBD-CGD-O1D
3	A	202[B]	HEM	CAD-CBD-CGD-O2D
3	C	202	HEM	CAA-CBA-CGA-O1A
3	A	202[A]	HEM	CAA-CBA-CGA-O1A
3	A	202[A]	HEM	CAD-CBD-CGD-O1D
3	D	202	HEM	CAD-CBD-CGD-O2D
3	A	202[B]	HEM	CAA-CBA-CGA-O2A
3	A	202[A]	HEM	CAA-CBA-CGA-O2A
3	A	202[B]	HEM	CAA-CBA-CGA-O1A
3	C	202	HEM	CAD-CBD-CGD-O2D
3	C	202	HEM	CAD-CBD-CGD-O1D
4	C	203	MPD	C2-C3-C4-C5
4	A	203	MPD	C2-C3-C4-O4

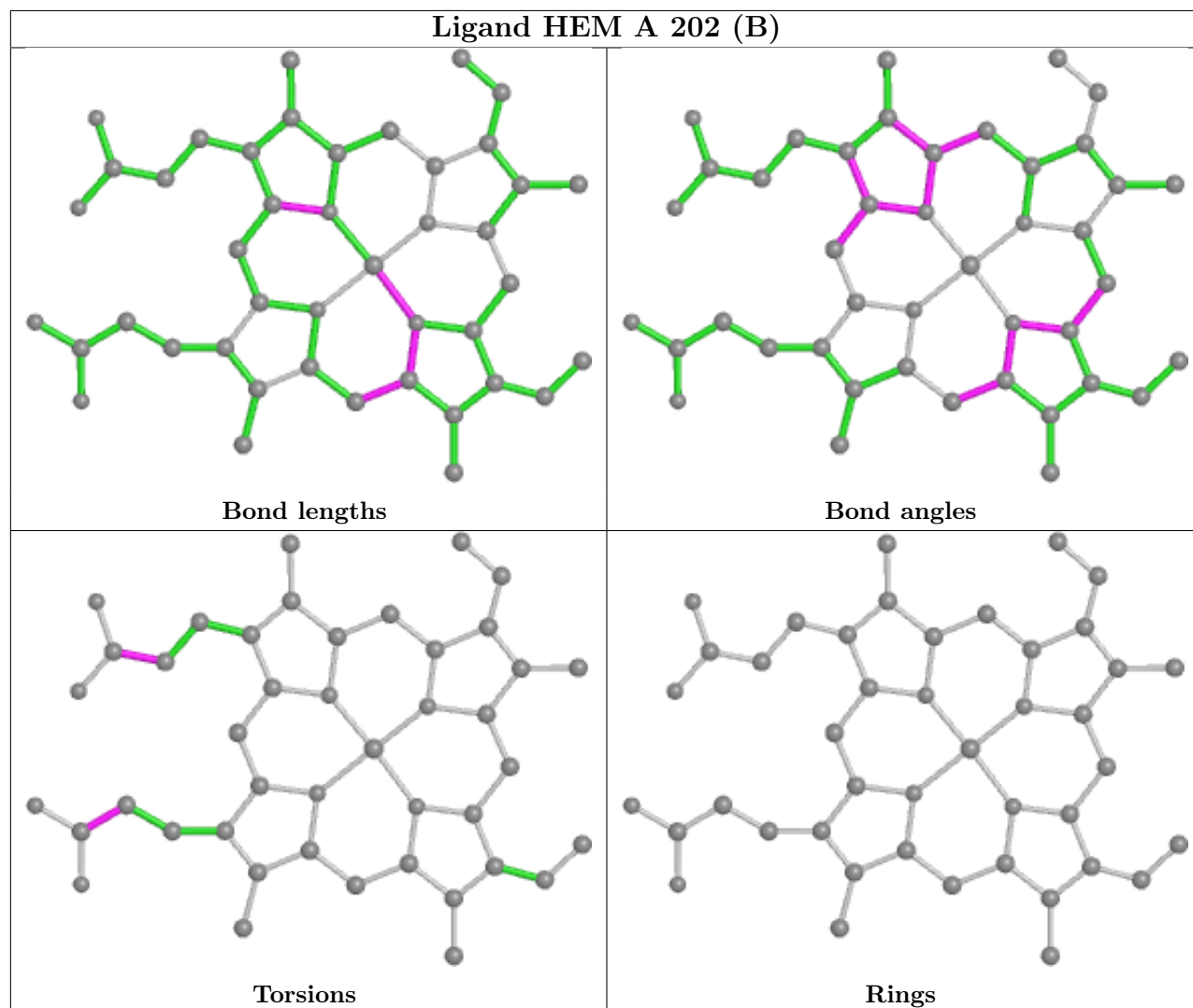
There are no ring outliers.

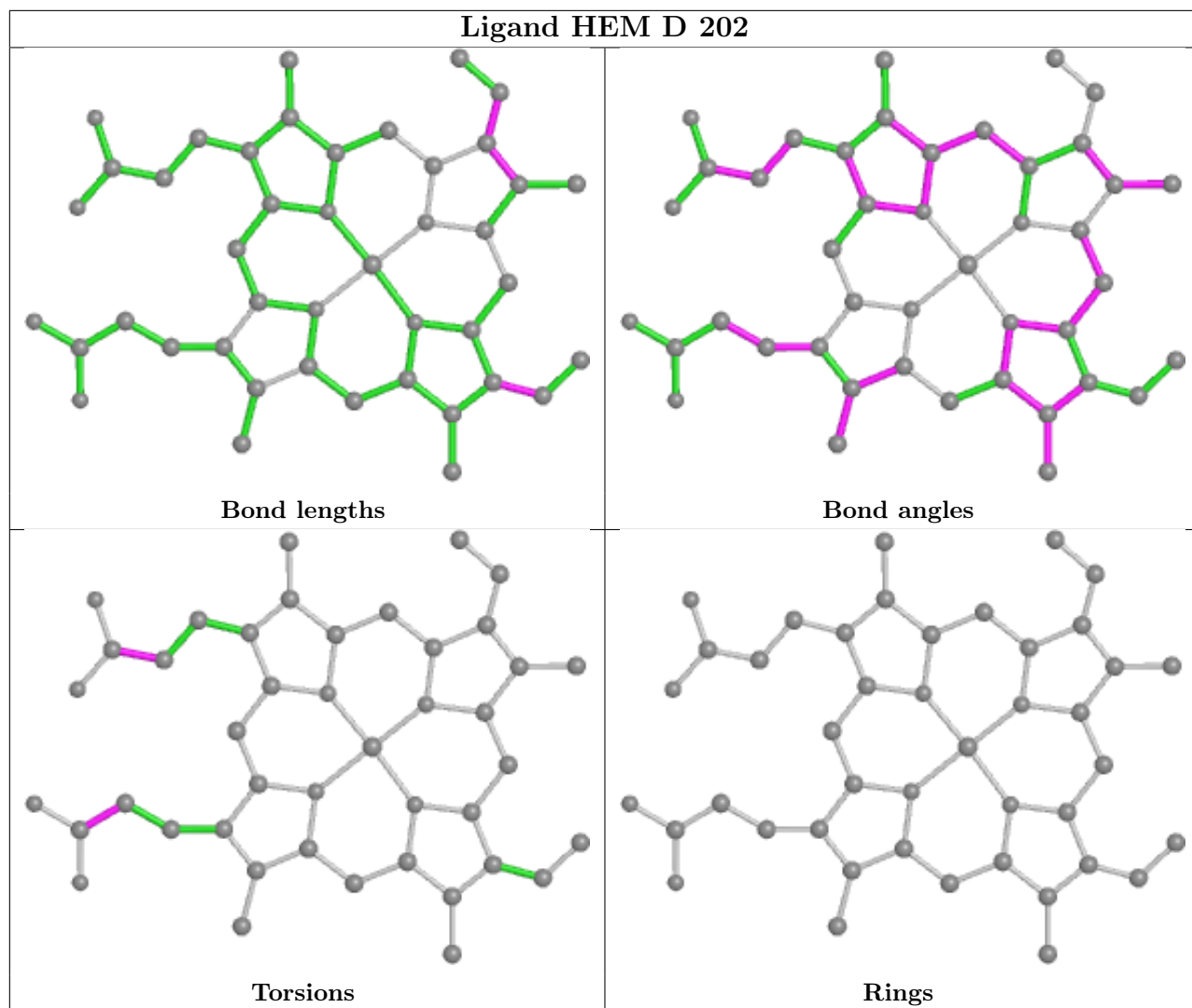
1 monomer is involved in 1 short contact:

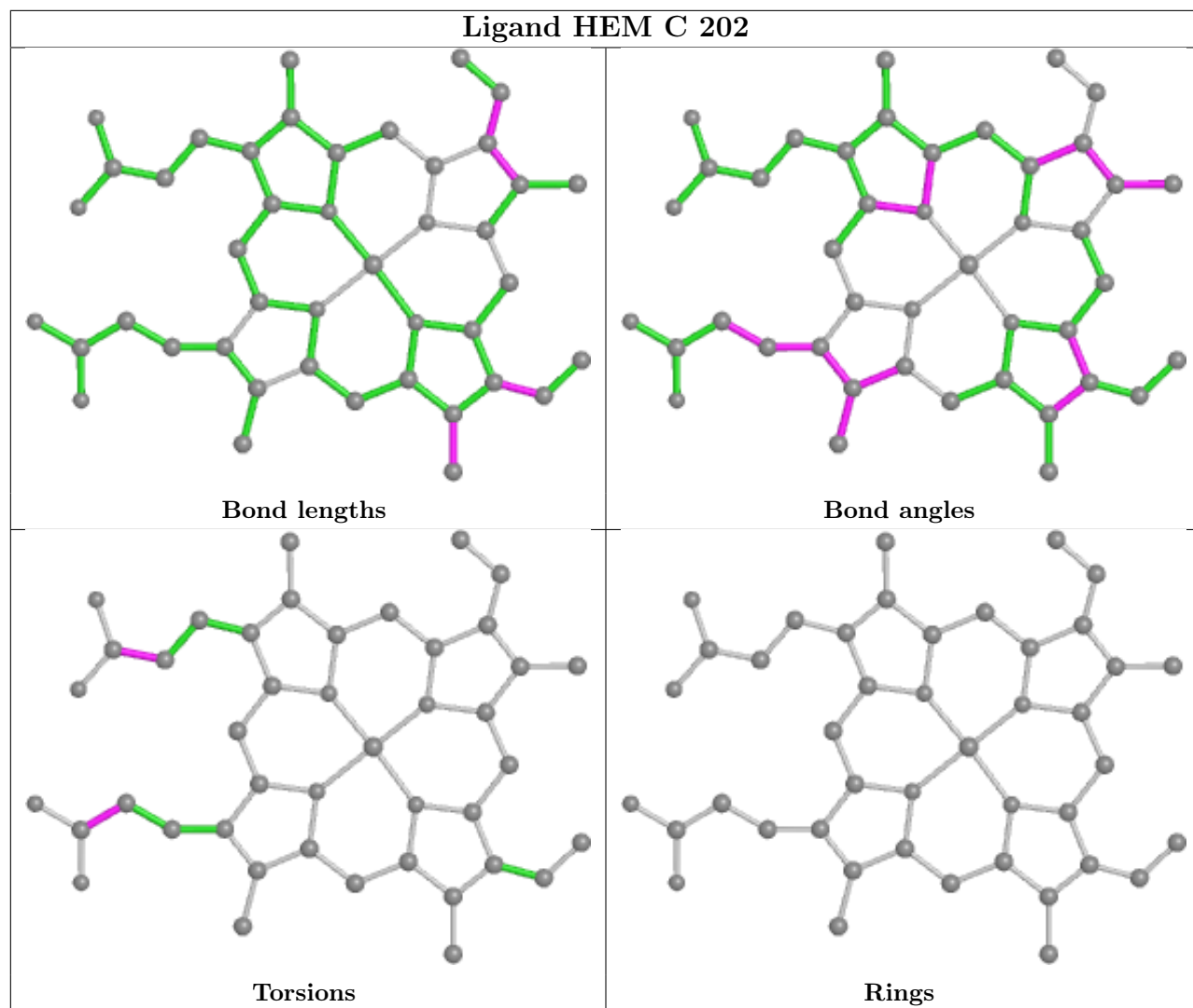
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	203	SO4	0	1

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

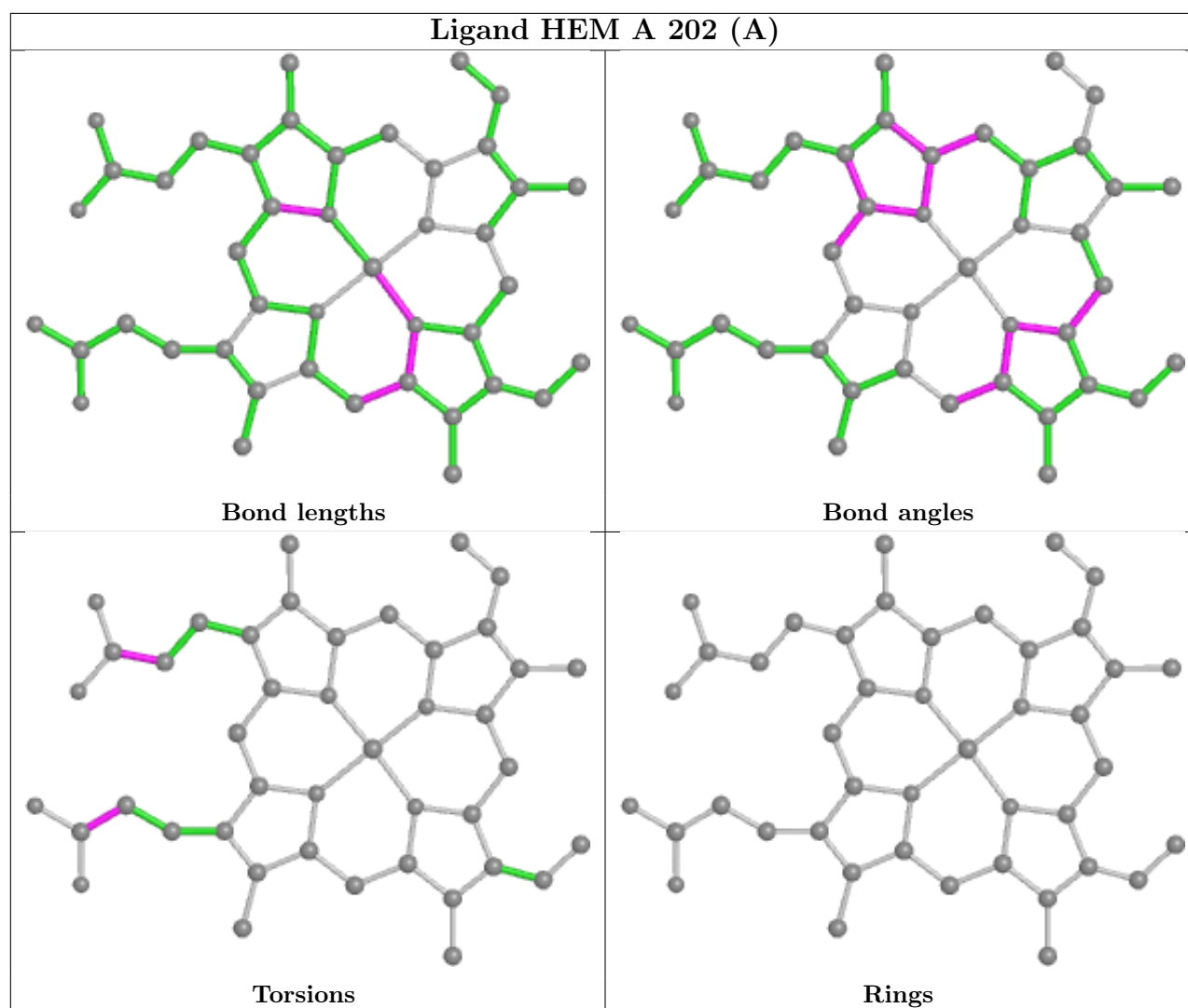
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











#### 4.7 Other polymers [i](#)

There are no such residues in this entry.

#### 4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 5 Fit of model and data [i](#)

### 5.1 Protein, DNA and RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

### 5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

### 5.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

### 5.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

### 5.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.